

tert-Butyl nitrite

540-80-7 | DTXSID10202316

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 39.0 °C

Global applicability domain: Inside

Local applicability domain index: 5.88e-01

Confidence level: 6.72e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Acetoxime

Measured: 61.0

Predicted: 37.2

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Acetamide, N-acetyl-N-methyl-

Measured: -25.0

Predicted: -28.7

[Image not found](#)

2,3-Butanedione-2-oxime

Measured: 76.8

Predicted: 74.5

[Image not found](#)

Trimethadione

Measured: 46.0

Predicted: 51.8